

**RECEIVED**  
**CENTRAL FAX CENTER****APR 18 2007****REMARKS**

Claims 1 to 122 are before the Examiner. New claims 123 to 132 are added. Claims 1 to 26, 28 to 43, 53, 57 to 59, 75 and 76 have been cancelled. Claims 27, 44 to 52, 54, 55, 56 and 60 to 122 are pending. Applicant respectfully requests that the instant application be reconsidered in light of the above amendments and the following remarks.

Claims 48, 54 to 56, 64 to 68, 70 to 74, 77 to 79 and 121 are amended

New claims 123 to 132 are added. Applicant also notes these embodiments of Applicant's compounds do not fall within the specific language of the count 103,819 drawn from Dow's patent applications. Specifically, claims where J is oxygen do not fall within the language describing the compound. Claims where the Cp group is fluorenyl do not fall within the language describing the compound. Claims where Z is carbon do not fall within the language describing the compound. Claims where R' or R have more than 10 carbon atoms do not fall within the language describing the compound.

Applicant thanks the Examiner for entering the numerous new claims presented in the previous office action.

**Restriction under 35 USC § 121**

Claims 27, 44 to 56 and 60 to 122 have been subjected to a restriction requirement to one of the following inventions:

Invention I: Claims 27, 44-56, 60-82 and 122, drawn to compounds, classified in class 556, subclass 53; and

Invention II: Claims 83-121, drawn to a polymerization process, classified in class 526, subclass 161.

The Office Action constructively elects Invention I based on original presentation for prosecution on the merits.

Applicant confirms the election of Invention I, with traverse.

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In particular, as noted in the U.S. Patent and Trademark Office Manual of Patent Examining Procedure §803, “[i]f the search and examination of all the claims in an application can be made without serious burden, the examiner must examine them on the merits, even though they include claims to independent or distinct inventions” (emphasis added).

Applicant respectfully submits that the search and examination of all of the claims in the application can be made substantially without burden, and certainly without serious burden, since the Examiner has already searched and examined claims from both asserted Inventions I and II.

For example, present claim 105 is very similar, though slightly narrower in scope (except of course for the presence of the Ti in the genus “M”) to (canceled) claim 44 of U.S. application serial no. 07/676,690. It is noted that claim 44 was searched, examined and allowed in the 07/676,690 application. Thus, the only outstanding issues regarding the patentability of present claim 105 should be the same as those discussed below for the product claims regarding the inclusion of Ti in the genus.

Applicant also notes that Invention II has already been searched by the Examiner for the same invention in US application serial no. 11/387,217, filed March 23, 2006. In fact, in the Office Action dated February 23, 2007, the 11/387,217 application, the Examiner states that present claims 83-121 claim “substantially the same process of polymerization” as that of claims 1-16 of the 11/387,217 application. Furthermore, in the 11/387,217 application, other than double patenting rejections, the only rejection is based on “the lost count in Interference No. 103,819,” which relates to exactly the same unusual issue that is addressed in the outstanding Office Action in the present application. Thus, it makes the most sense to address this issue, with regard to Inventions I and II, both at the same time.

Thus, as claims from both Inventions I and II have already been searched and examined, and because the unusual issues with regard to patentability of both Inventions I and II should be considered at the same time, it is respectfully submitted that it would not require undue burden to examine both Invention I and II in this application. Additionally, the Examiner alleges that the inventions differ as product and process of use. Applicant respectfully submits that regardless of the classification system noted above, the

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Examiner will have to search the same art, for both inventions of Group I drawn to polymerization catalysts and of Group II drawn to a polymerization process, and rarely is one described without describing the other. Thus, it is more efficient and cost effective if both are searched and examined at the same time, particularly since, as discussed above, they have already been searched and examined.

Thus Applicant respectfully submits that it would not require an undue burden for the Examiner to search and examine both Inventions. To the extent that a minor additional burden would be assumed by the Examiner in withdrawing the Restriction Requirement and acting on all the claims, the possible additional adverse impact on Applicant, if the restriction is not withdrawn, is enormous. This is because any divisional application filed at this point would have a severely limited patent term. While rejoinder of the claims is assured when the claims of Invention I are eventually found to be allowable, if the claims were rejoined now, the claims of Invention II would be found to be allowable, or at least rejected only on grounds related to the inclusion of titanium.

For all the above reasons, Applicant respectfully requests withdrawal of the restriction requirement.

Furthermore, in the event the Examiner does not withdraw the restriction requirement, Applicant requests rejoinder of the claims under MPEP § 821.04(b).

#### Claim Objections

Claims 64, 66, 68, and 70-74 are objected to because Hr should be Hf. Claims 48, 64-68, 70-74, and 121 have been amended to change Hr to Hf. Applicant respectfully requests that the rejection be withdrawn.

#### Claim Rejections -Obviousness Type Double Patenting

Claims 48-56 and 60-63 and 64-82 are rejected as unpatentable under the judicially created doctrine of obviousness type double patenting over US 7,041,841, US 5,621,126, RE 37,788 and US 6,617,466.

Applicant respectfully disagrees with the above obviousness type double patenting rejections and respectfully submits that claims 48-56 and 60-63 and 64-82 are

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not obvious over the four cited patents and the rejections should be withdrawn. In the instant application, the Examiner has agreed the two-way test for obviousness type double patenting is to be applied.

Obviousness-type-Double Patenting over US 7,041,841

Applicant notes that on May 23, 2005 a terminal disclaimer (copy attached) was filed in USSN 07/973,261 (now US 7,041,841) disclaiming the terminal portion of US 7,041,841 over the instant application. The doctrine of obviousness type double patenting was developed to prevent unjustified extensions of patent term. Since the instant application and US 7,041,841 will expire no later than the expiration date of the instant application and the terminal disclaimer in US 7,041,841 already requires common ownership, there is no need for another terminal disclaimer in the instant application. Applicant respectfully submits that the obviousness type double patenting rejection should be withdrawn.

Additionally, claims 1, 2, 3, and 5 of US 7,041,841 are directed toward symmetrically substituted (e.g.  $x = 2$  or 4) Hf and Zr compounds useful for producing polymers having greater stereoregularity. Specifically the special combination of Hf or Zr with  $x$  being 2 or 4 has an unexpected technical effect of enhanced stereoregularity in polypropylene (see column 25, line 29). This is particularly true when one considers that titanium is usually the preferred species for the instant mono-Cp catalysts. Therefore, claims 1, 2, 3, and 5 of US 7,041,841 are not obvious from the instant application. Likewise the instant application is not obvious from the claims in US 7,041,841. Claims limited to Hf and Zr do not suggest the full scope of the instant claims of Hf, Zr, and Ti, especially when one considers that Ti is not preferred for propylene catalysts. Likewise claims limited to  $x = 2$  and 4 do not suggest  $x$  of 1, 2, 3 or 4. Thus, Applicant submits that the instant application is not obvious from the claims in US 7,041,841. Since neither prong of the two-way obviousness test has been met, Applicant requests that the obviousness type double patenting rejection be withdrawn.

Obviousness-type-Double Patenting over US 5,612,126 and its reissue RE 37,788

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US 5,612,126 and its reissue RE 37,788 are directed toward specific catalyst compounds having the ability to produce ethylene alpha -olefin copolymers of high molecular weight with high levels of alpha-olefin comonomer incorporation and at high levels of catalyst productivity (see col. 1, lines 40-47 of '126). Specifically catalyst compounds having an R' group that is a 1° or 2° carbon atom bonded to the J atom have an *unexpected technical effect* of achieving high levels of alpha-olefin comonomer incorporation at high molecular weights. As evidence of this unexpected effect please see Table 1 in US 5,612,126 and its reissue RE 37,788. Specifically, when we compare examples 80 to 82 and 77 to 79, we see that the comonomer incorporation is significantly greater, when a 1° or 2° carbon is bonded to J versus a 3° carbon, and the molecular weights are increased. Normally in coordination polymerization one expects that high comonomer content depresses molecular weight and vice versa. It is highly unusual that one could get both high comonomer and high molecular weight at the same time. This also has the production benefit that one needs less comonomer in the reactor to produce a same density product as previous catalyst. This could result in significant monetary savings. This specific combination is neither disclosed nor suggested in the instant claims. Therefore the claims in '841 are not obvious from the instant claims.

Furthermore, please note that US 5,055,438 is listed on the face of US 5,612,126 and its reissue RE 37,788 as having been considered by the Examiner and found to NOT make the inventions claimed therein obvious. The instant application is a divisional of US 5,055,438 and thus has the SAME specification. If the USPTO has found the claims of US 5,612,126 and its reissue RE 37,788 patentable over the entire disclosure of US 5,055,438, then it logically follows that US 5,612,126 and its reissue RE 37,788 are patentable over the instantly claimed invention. Thus, Applicant respectfully submits the obviousness type double patenting rejection should be withdrawn.

In addition, Applicant notes that RE 37,788 is the reissue of US 5,612,126. Applicant was required to surrender the ribbon copy of US 5,612,126 in order to obtain the reissue, and once a patent is reissued, the original granted patent is no longer in force. See 37 CFR § 1.178 which states *[u]ntil a reissue application is granted, the original patent shall remain in effect.*" emphasis added. Therefore, Applicant respectfully submits

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that since US 5,612,126 is no longer in force, a terminal disclaimer is neither proper nor necessary.

Obviousness-type-Double Patenting over US 6,617,466

Claims 1-20 of US 6,617,466 are directed toward a process to produce a defined catalyst compound comprising reacting a Group IV B transition metal halide with a salt containing an anion of the formula  $((C_5H_4-xR_x)-T-(JR'_{2-2}))^{-2}$  and either two cations from Group I A or one cation from Group II A of the Periodic Table of Elements. As the Examiner is aware a two-way obviousness test is required in the instant situation. Applicant submits that while it might be obvious that the method claimed in '466 would produce the instantly claimed compounds, it is NOT obvious that one would use the claimed method to obtain the instantly claimed compounds. There are other methods that can be used to obtain the instantly claimed compounds. Further it is also not obvious that any given production process will produce a compound capable of polymerizing olefins. Thus, Applicant respectfully submits that the two-way obviousness test has not been met and requests that the rejection be withdrawn.

Rejection under 35 USC § 102(e)

Claims 64, 66 and 68 are rejected under 35 USC § 102(e) as being anticipated by Example 1 of Tomotsu (US 5,276,117) which the Examiner suggests discloses  $Me_5CpTi(OMe)_3$  with 1/2 molar equivalent of ethylene glycol. Applicant respectfully disagrees and notes that in Example 1 Tomotsu specifically contacts the ethylene glycol with the methylalumoxane activator *prior* to contacting with the  $Me_5CpTi(OMe)_3$  (see column 6, line 58-59 which states "*After addition of ...ethylene glycol...*"). The ethylene glycol is a modifier for the MAO activator that reacts with the MAO *prior* to the addition of the  $Me_5CpTi(OMe)_3$ . Note that this is a preferred method of practicing the invention (column 5, line 5-8). An even more preferred method is to react the ethylene glycol with the components that make the MAO as one makes the MAO. (see column 5, line 9, et seq.)

Additionally even if the components were added "successively" (A) plus (B) then plus (C) (i.e.,  $Me_5CpTi(OMe)_3$  +MAO, then +ethylene glycol) as suggested at column 5,  
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line 6, the result would still not be Applicant's claimed invention. Those of ordinary skill in the art traditionally use a significant excess of alumoxane when working with metallocene type compounds. This significant excess would use up most, if not all, of the ethylene glycol, as Tomotsu intends it to do. Note that in Example 1, Tomotsu uses 6 mmol of aluminum (e.g. alumoxane) versus 0.03 mmol of ethylene glycol and 0.06 mmol of  $\text{Me}_5\text{CpTi}(\text{OMe})_3$ . This is 200 times more alumoxane than ethylene glycol on a molar basis, 100 times more on an equivalent basis. Note also that twice as much  $\text{Me}_5\text{CpTi}(\text{OMe})_3$  is present as relative to the ethylene glycol. Further, even if the ethylene glycol could find the  $\text{Me}_5\text{CpTi}(\text{OMe})_3$  ("Cp compound") to react with, the Cp compound will have been activated by the MAO already, meaning that one of the OMe groups would no longer be attached to the Ti. If the ethylene glycol could get to the activated Cp compound and did react with it, this would still not make Applicant's claimed invention because there would not be two anionic leaving groups ("Q" groups) and a Lewis base bonded to the metal as required in the claims. Thus even "successive" addition would not produced the claimed invention.

Applicant respectfully submits that when Tomotsu is read in full, that it is clear that no where within the four corners of the document is it disclosed or suggested that the ethylene glycol (component (C)) be bonded to the Ti compound prior to combination with any activator. Thus, Tomotsu does not disclose Applicant's claimed invention requiring a Lewis base to be bonded to the metal (the arrow in the formula represents a dative bond). In light of the above, Applicant respectfully requests that the rejection under 35 USC § 102(e) over Example 1 of Tomotsu be withdrawn.

#### Relationship Of The Ti, Zr, Hf Genus And The Ti Species

The count in the 102,953 interference (which the instant application was involved in) was directed to the genus of mono-Cp compounds having Ti, Zr, or Hf.

ExxonMobil won the interference and was awarded priority for the count.

Dow believed that the Ti species has unexpected results as compared to the genus of compounds having Ti, Zr, or Hf that make the Ti species separately patentable from the genus. Dow filed a motion in the '953 interference to this effect and requested a separate interference. This motion was denied.

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Dow made a similar motion in the 102,954 interference (Motion 13). The count in that interference was to a process to polymerize olefins comprising using a catalyst system comprising a specific Mono-Cp compound and alumoxane, where the metal in the Mono-Cp compound was Ti, Zr or Hf. Dow's motion to include a count limited to titanium was denied (see page 61, of the Final Decision in 102,954, (Paper 681)).

Dow made another similar motion in the 102,955 interference. (Motion 12, 102,955) The count in that interference was to a catalyst system comprising a specific Mono-Cp compound and alumoxane, where the metal in the Mono-Cp compound was Ti, Zr or Hf. Dow's motion to include a count limited to titanium was initially denied. The request, however, was later referred to the *ex parte* Examiner David Wu who found an interference in fact regarding a specific catalyst system (see Interference Initial Memorandum attached to the Declaration of Interference, Paper 17 103,819). The PTO agreed with Dow's view that a catalyst system containing the Ti species is separately patentable from a catalyst system containing the genus of compounds having Ti, Zr, or Hf and declared the 103,819 interference. The count in the '819 interference was directed to a catalyst system comprising mono-Cp compounds having Ti and alumoxane. (see Papers 17 and 20, Interference 103, 819.)

ExxonMobil conceded the '819 interference, and the PTO awarded priority for the count to Dow. (see Paper 168, 103,819 Interference.)

The relationship between the genus of compounds having Ti, Zr, or Hf and the Ti species depends on whether the genus was invented before or after the species. If the species was invented before the genus, then the species would anticipate the genus, and the genus would not be patentable. If, however, the genus was invented before the species, and the species was separately patentable from the genus, then both the genus and the species can be patentable. This very situation was remarked upon by the Federal Circuit in *Eli Lilly & Co. v. Bd. Of Regents Of The Univ. Of Washington*, 334 F.3d 1264, 1268 (Fed. Cir. 2003). Specifically *Eli Lilly* confirmed the acceptability of the Patent Office's practice of requiring a two-way test for determination of "same patentable invention" for declaration of interferences. As the court discussed the consequences of the two-way test, they acknowledged that if the genus was invented first, it could lead to a situation where both the genus and species were patentable, e.g...

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The Director, in an amicus brief, interprets § 1.601(n) as requiring a two-way test to determine whether two parties claim the "same patentable invention." The two-way test assures that an interference proceeding will be conducted only when warranted. The Director's approach rejects a wooden requirement under the over-inclusive one-way test of declaring an interference proceeding where a species claim allegedly anticipates a genus claim. If the interference proceeding, however, leads to a conclusion that the genus claim was invented first, it is possible that both the genus and the species are separate patentable inventions. Thus, the Director's two-way test avoids the proliferation of unnecessary, wasteful interference proceedings concluding that both parties are entitled to patents in situations in which the claimed inventions do not define the same patentable invention, but merely overlap in scope. This is the clear application of discretion that is inherent in the authority granted pursuant to 35 U.S.C. § 135(a) of the statute. *Eli Lilly & Co. v. Bd. Of Regents Of The Univ. Of Washington*, 334 F.3d 1264, 1268 (Fed. Cir. 2003) (emphasis added).

Applicant submits that this is the situation in the instant Application. Specifically ExxonMobil's proofs during the interference showed conception and reduction to practice of Hf and Zr and conception of Ti before Dow's conception and reduction to practice of Ti. APJ Downey agreed with regard to the compound and process to polymerize, however Dow had data to show Ti catalyst systems conceived and reduced to practice *after* ExxonMobil's proofs had, *inter alia*, better activities than Hf and Zr. Thus, the Applicant's Hf, Zr, Ti genus was invented first. Dow's specific Ti species was invented second and was arguably patentable over the genus. Hence, under the logic set out *Eli Lilly* both are entitled to patents.

#### Rejection Over The Lost Count In Interference 103,819

Claims 48-50, 53-56, 61, 63-65, 67-75, and 77-82 are rejected under 102(g) over the lost count in the 103,819 interference.

In awarding priority to ExxonMobil in the '953 interference, the PTO determined that ExxonMobil was the first inventor of the subject matter of the count – the genus of mono-Cp compounds having Ti, Zr, or Hf. In making this determination, the PTO also necessarily determined that ExxonMobil invented the genus of compounds having Ti, Zr, or Hf before Dow invented the species of compounds having only Ti. Otherwise, Dow's invention of the Ti species would have anticipated the genus of compounds having Ti, Zr, or Hf, and ExxonMobil could not have been awarded priority in the '953 interference.

The history of the '953 and '819 interferences and the claims to the genus of compounds having Ti, Zr, or Hf that Applicant now seeks in the present application is exactly the scenario that the Federal Circuit discussed in *Eli Lilly* above. In this scenario – where a first inventor invents a genus, a second inventor invents a separately patentable species that falls within the genus, and the genus was invented before the species – the Federal Circuit observed that both inventors can receive patents. This is why both Applicant's claims and Dow's '819 count are patentable and both can issue as patents without violating the Examiner's "...fundamental concept that a genus is never patentable over a narrower species."

Furthermore Dow presented the Examiner's very argument in it's FINAL HEARING BRIEF at Section XIV, page 230 when Dow stated "*The Board should also issue a statement in its decision to the effect that Canich is not entitled to any claim that embraces any genus that includes compounds made from titanium.*" APJ Downey denied Dow's Section XIV request (Motion 12) and did *not* adopt Dow's suggested statement quoted above. Instead APJ Downey ruled "Jo Ann M. Canich, the junior party, is entitled to a patent containing claims 2, 4-6, 25, 26, 35-41, 44 and 45 of their application corresponding to Count 2." (see page 53 of the decision in the '953 interference (paper no. 578), previously submitted). Note that APJ Downey's language states that Canich is *entitled to a patent... corresponding to Count 2*. Count 2 clearly includes titanium, zirconium and hafnium in the definition of M. Judge Downy had specifically been presented with the Examiner's argument and ruled against it.

Consequently, Applicant submits that the USPTO has already decided these issues in the lengthy, time consuming and expensive '953, '954 and '955 interferences and that the USPTO is not a liberty to disregard these judgments and instead must follow these judgments by withdrawing the rejection over the '819 count and passing Applicant's claims to allowance.

Furthermore, Applicant respectfully submits that the lost count in the '819 interference was to a catalyst system, which is a separate patentable invention from the claims for the compounds and process claims that Applicant now seeks. The PTO

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recognized that the compound, the process and the catalyst system are separate patentable inventions by declaring separate interferences: the '953 interference was directed to a compound, the '954 was directed to a polymerization process, and the '955 interference was directed to a catalyst system. Since the count in '819 is separately patentable, Applicant submits it should not be cited against the instantly claimed inventions.

Furthermore, MPEP § 2308.03(a) states "A party is barred (estopped) from raising an issue if the party lost on the issue during the interference. A party may lose on one issue, yet not lose on a different issue. Example The applicant lost the interference on a count drawn to a compound, but the opponents lost on a count drawn to methods of using the compound. The applicant may continue to pursue claims to the method of using the compound, but not claims of the compound itself." In light of MPEP § 2308.03(a) Applicant submits that the lost count in '819 was to the *catalyst system* (i.e. a transition metal compound and an alumoxane), and the successful count in the instant application ('953 interference) was not to catalyst system, but to the compound. Likewise the successful count in the '954 interference was to the polymerization process, not a catalyst system. Both of these successful counts define different patentable inventions that fit the example in MPEP § 2308.03. Thus, Applicant further submits that the claims to the compound and the polymerization process are not estopped and under MPEP § 2308.03 and thus should not be rejected over the lost count in the 103,819 interference.

In light of the above Applicant respectfully request that the Examiner withdraw the rejection rejecting the claims over the lost count in Interference 103,819.

Applicant notes that USSN 11/729,987, filed March 29, 2007 (Attorney Docket number 89B010A6) contains claims to a catalyst system and submits that perhaps the lost count in interference No. 103,819 should be addressed in that application rather than the instant application.

#### Claim Rejections Under 35 USC § 103(e)

Claims 64-69 and 122 are rejected under 35 USC § 103(a) as anticipated by Examples 2 to 12 of Campbell (US 5,045,517) which the Examiner suggests discloses a  
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variety of Cp complexes, including Cp-Ti-phenoxy dichloride and CpTi-tris-dimethylamide. The Examiner acknowledges that L is missing, but suggests that one would be motivated to add L because Campbell suggests addition of alcohols at Column 2, line 31-39. Applicant respectfully disagrees. Applicant's claimed invention requires that a Lewis base be bonded to the titanium. It is known to one of ordinary skill in the art that the arrow in the Applicant's formula represents a dative bond. As support for the position that arrows are used to represent dative bonds, please see page 8, of *Introduction to Organic Chemistry*, 2nd ed., Streitwieser, Jr. and Heathcock, Macmillian Publishing Co., Inc. New York, 1981 (copy attached), which states "*The use of a 'dative or coordinate covalence' bond is sometimes convenient. In this convention, an arrow represents a two-electron bond in which both electrons are considered to 'belong' to the donor atom for the bookkeeping purposes of assigning formal charges.*" Thus it is clear that one of ordinary skill in the art would understand the Lewis base is bonded to the metal. In contrast Campbell does not describe a titanium compound where the Lewis base is bonded to the metal. Instead Campbell describes a situation where the Lewis base is loosely associated with the compound by Van der Waals forces. Van der Waals forces are so weak they are not considered bonds, they are considered weak forces. Further, it is common for other molecules to be associated with or trapped in the crystal structure of another compound, yet not bound to that compound. For example, please see page 93-94 of *Concepts and Models of Inorganic Chemistry*, Bodie E. Douglass, and Darl H. McDaniel, Blaisdell Publishing Company, a division of Ginn and Company, Waltham, Massachusetts, 1965, where clathrate compounds are described. In the example described on page 93, the benzene molecule is associated with and trapped in the crystal structure of the nickel molecule, but not bonded to it. Applicant respectfully submits that Campbell teaches such a situation. Campbell at column 2, line 35, et seq. states "*An example includes such complexes additionally incorporating one or more molecules of any nature in the crystal structure, such as alcohol molecules associated with the crystal structure via Van der Waals forces.*" Applicant respectfully submits that alcohols associated by Van der Waals forces in the crystal structure of the compound are not the same thing as a Lewis base that is datively bonded to the metal compound. Further, nothing within the four corners of Campbell suggest bonding a Lewis base to the

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compound. Thus, Applicant respectfully submits that Campbell does not disclose or suggest Applicant's claimed invention and requests that the rejection be withdrawn.

Accordingly, Applicant respectfully requests the rejections to the claims be removed, and the claims, as amended, be passed to allowance.

Please charge any deficiency in fees or credit any overpayments during the entire pendency of this case to Deposit Account No. 05-1712. Please also charge any petition fees, including fees for extensions of time necessary for the pendency of this case or copendency of this application with another application at any time to Deposit Account No. 05-1712.

Respectfully submitted,

April 18, 2007  
Date:

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Attachments: Terminal disclaimer filed in USSN 07/973,261 (now US 7,041,841)  
Page 8, *Introduction to Organic Chemistry*, 2nd ed.  
Page 93 of *Concepts and Models of Inorganic Chemistry*

# **Introduction to Organic Chemistry**

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**Andrew Streitwieser, Jr.  
Clayton H. Heathcock**

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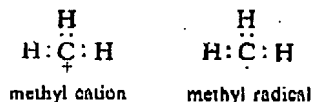
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Structure  
and Bonding

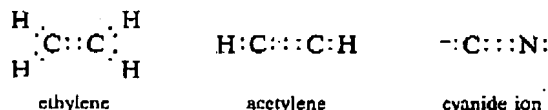
electrons are spread over the entire molecule. However, this method of assigning formal charges does keep strict account of the total numbers of electrons and charges present and, when used with care, it helps to interpret chemistry. For example, the formal charge of  $-1$  assigned to the oxygen of methoxide ion helps to explain why this ion is a strong base that readily adds a proton to the oxygen.

The example of sulfate ion is more complex. Some students tend to write this ion as  $^- \ddot{\text{O}} : \ddot{\text{O}} : \text{S} : \ddot{\text{O}} : \ddot{\text{O}} : ^-$ , an arrangement that has the proper number of valence electrons and a less complex formal structure assignment. However, sulfate ion is known experimentally to have each oxygen bound to sulfur in an equivalent manner.

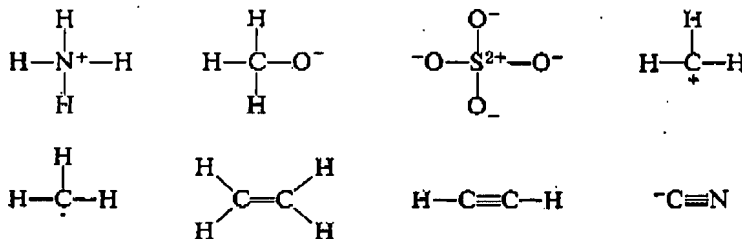
When a species has an incomplete octet, it is usually unstable or highly reactive. Examples are methyl cation and methyl radical.



Multiple bonds are handled in a straightforward manner.

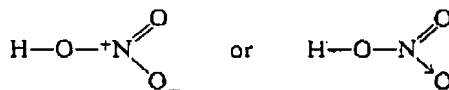


A further simplifying convention is to replace each electron-pair bond by a line. For convenience, electron pairs are frequently omitted.



In these symbolic representations, the lone-pair electrons are understood to be present and their presence is signified by appropriate formal charges. This is another reason for assigning formal charges properly. *The use of such symbols is widespread in organic chemistry, and practice in reading and writing these electronic representations cannot be overemphasized.* The simplified symbols correspond to an earlier notational system proposed by August Kekulé. Accordingly, such symbols, in which each electron-pair bond is represented by a line and the lone-pair electrons are omitted, are frequently called **Kekulé structures**.

The use of a "dative" or "coordinate covalence" bond is sometimes convenient. In this convention, an arrow represents a two-electron bond in which both electrons are considered to "belong" to the donor atom for the bookkeeping purpose of assigning formal charges.



This type of symbolism finds most use in representing ligands in inorganic complexes and will rarely be used in this text.

## EXERC

ing all of

(a) chlor

(c) hydr

(e) ozon

(g) cyan

## 2.3

## Geom

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# *Concepts and Models of Inorganic Chemistry*



ENCES

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by the covalent molecules by van der Waals forces. They can be pictured as spheres of a certain radius. There is a limit to the radius of the sphere. The radius of the sphere is greater than the radius of the atom. The attraction between the two

forces between the spheres. The rigidly spherical molecules are symmetrical on a sphere. The force of attraction between the atoms or molecules

between molecules is increasing molecular weight. It is not *per se* without effect on the boiling point for many fluorine atoms. The corresponding low boiling points of their interaction

ions

for a molecule induced dipole

the distance between the nuclei exclusion principle distance have

### Clathrate Compounds

93

in the symmetrical molecule. The inert gases form hydrates that could be the result of dipole-induced dipole interactions, since the more stable hydrates are formed by the larger and more polarizable inert gas atoms. These hydrates are probably more properly regarded as clathrate compounds.

There are few clear-cut cases of ion-induced dipole interactions because in situations where such attractions might occur there are other more important forces present. Thus, the interactions between ions and a nonpolar molecule in an ionic medium would be much less important than the ionic interactions. The greater stability of ammonia complexes of some metals as compared to the aquo (water) complexes can be explained as the result of the greater polarizability of ammonia. Thus the total dipole moment, permanent plus induced, of ammonia in such complexes is greater than that of water in similar complexes (see p. 347).

### Ion-Dipole and Dipole-Dipole Interactions

Ions attract the polar water molecules very strongly to form hydrated ions. The hydration energy released provides the energy required for the separation of the ions from the ionic crystal. The effect of the attraction between dipoles can be observed in the boiling points of  $\text{NF}_3$  ( $-129^\circ\text{C}$ ) and  $\text{OF}_2$  ( $-144.8^\circ\text{C}$ ) compared to  $\text{CF}_4$  ( $-161^\circ\text{C}$ ), which has zero dipole moment.

### Clathrate Compounds

There are a number of compounds for which the composition appears very strange and unaccountable in terms of the usual bonding forces. The compound  $\text{Ni}(\text{CN})_2(\text{NH}_3)_6\text{C}_6\text{H}_6$  was originally thought to be a coordination compound in which there were four groups bonded to the nickel, including the benzene molecule. It has been shown that the compound has a very interesting structure in which half of the nickel ions have a coordination number of six because ammonia molecules are coor-

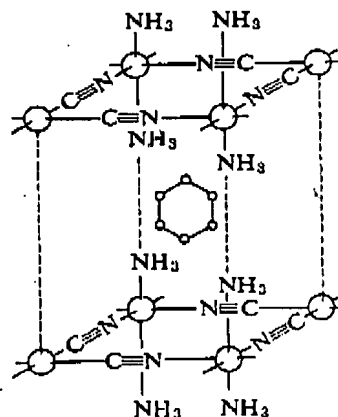


FIGURE 2.36. The  $\text{Ni}(\text{CN})_2(\text{NH}_3)_6\text{C}_6\text{H}_6$  clathrate compound (from J. H. Rayner and H. M. Powell, J. Chem. Soc., 1952, 319).

minated above and below the plane. The six-coordinate nickel ions are bonded to the nitrogen of the  $\text{CN}^-$ . The benzene molecule is trapped in the "holes" in the lattice because it just fits in (Figure 2.36). Compounds in which a molecule is trapped in the "cage" of the crystal lattice are called *clathrate compounds*. Hydroquinone forms a series of compounds, which approach the composition  $(\text{C}_6\text{H}_6\text{O}_2)_n \cdot \text{Y}$ , where Y can be HCl, HBr,  $\text{H}_2\text{S}$ ,  $\text{SO}_2$ , etc.

Clathrate compounds have become important in the separation of isomeric hydrocarbons. Urea and thiourea have been widely used as the solid phase and recently inorganic complexes have been used for separations such as the recovery of *p*-xylene from either gasolines or from aromatic hydrocarbons of comparable molecular weights by single step operations.\*

The tendency for water molecules to form hydrogen bonds produces open structures in the solid state. The holes permit the formation of clathrate compounds of the type  $\text{Y} \cdot x\text{H}_2\text{O}$  (where Y may be Xe,  $\text{Cl}_2$ ,  $\text{Br}_2$ ,  $\text{SO}_2$ ,  $\text{CHCl}_3$ , etc., and  $x$  varies from about 6 to 17). Several tetraalkyl ammonium salts have been found to give hydrates in which the ions occupy cavities in some type of hydrogen bonded ice structure.† The compounds are of the type  $[(n\text{-C}_4\text{H}_9)_4\text{N}^+]_m \text{X}^{m-} \cdot my\text{H}_2\text{O}$  (where X is  $\text{F}^-$ ,  $\text{Cl}^-$ ,  $\text{Br}^-$ ,  $\text{CrO}_4^{2-}$ , etc., and  $y$  is approximately 32) and  $[(i\text{-C}_3\text{H}_7)_4\text{N}^+]_m \text{X}^{m-} \cdot my'\text{H}_2\text{O}$  (where X is  $\text{F}^-$ ,  $\text{Cl}^-$ ,  $\text{CrO}_4^{2-}$ , or  $\text{WO}_4^{2-}$  and  $y'$  is approximately 40). Each type of compound shown represents an isomorphous series. It is unusual to find an isomorphous series of compounds in which the same cation is combined with anions of different charge.

#### Radil of Atoms in Covalent Compounds

The bond length, the distance between two bonded atoms, in a covalent molecule such as  $\text{Cl}_2$  is taken as the sum of the covalent radii of the atoms. Thus the covalent radius of the chlorine atom is one half of the chlorine-chlorine distance (1.998 Å). The covalent radius for nonmetals is often called the atomic radius. The carbon-carbon bond distance in diamond (1.541 Å) is essentially the same as that in ethane (1.543 Å) and other saturated hydrocarbons. Carbon has a single-bond covalent radius of 0.77 Å. The covalent radii of carbon and chlorine can be combined to give 1.76 Å as the expected C—Cl bond distance, the same as that observed for  $\text{CCl}_4$ .

The single-bond radii of nitrogen and oxygen are not obtained from the bond lengths in  $\text{N}_2$  (1.10 Å) and  $\text{O}_2$  (1.208 Å) since these molecules contain multiple bonds. Instead the single-bond radii are obtained from the bond lengths in compounds such as hydrazine,  $\text{H}_2\text{NNH}_2$ , and hydrogen peroxide,  $\text{HOOH}$ . The radius of nitrogen obtained from  $\text{N}_2$  (0.55 Å) is the triple-bonded radius. A triple-bonded radius for carbon can be obtained from the carbon-carbon bond length in acetylene (1.21 Å). The triple-bonded radii of carbon and nitrogen can be combined to give the expected bond length  $(0.55 + 0.60 = 1.15 \text{ Å})$  for a  $\text{C}\equiv\text{N}$  bond as compared to the observed bond length 1.16 Å for  $\text{CH}_3\text{CN}$ . A double-bonded radius of carbon can be obtained from the carbon-carbon bond length (1.35 Å) in ethylene (see Table 2.2).

\* Schaeffer, W. D., W. S. Dorsey, D. A. Skinner, and C. G. Christian, *J. Am. Chem. Soc.*, 79, 5870 (1957) and F. V. Williams, *ibid.*, 79, 5876 (1957).

† McMullan, R., and G. A. Jeffrey, *J. Chem. Phys.*, 31, 1231 (1959).

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\* Schomaker, V., ar

N.		
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	C	
0.77		1.22
	Si	
1.15		1.50
	Ge	
1.21		1.60
	Sn	
1.42		1.80
" Huggins, M. L., J		